Updated Preliminary Response to Charge Questions and Sections of EPA's draft review documents from Members of the Science Advisory Board (SAB) Animal Feeding Operations Emissions Review Panel As of April 5, 2012

Purpose: This is an updated Preliminary Response to Charge Questions and updated comments on Sections of EPA's draft review documents from Members of the SAB Animal Feeding Operations Emissions Review Panel. This is related to the Panel's review of the following two EPA documents associated with EPA's emissions estimating methodologies for Animal Feeding Operations: a) "Draft - Development of Emissions Estimating Methodologies for Broiler Animal Feeding Operations" - February 2012 draft; and b) "Draft - Development of Emissions Estimating Methodologies for Lagoons and Basins at Swine and Dairy Animal Feeding Operations" - February 2012 draft. The first SAB Animal Feeding Operations Emissions Review Panel Meeting occurred on March 14-16, 2012.

Charge Question 1 Response and Comments on Section 7 of the Broiler Report

Charge Question 1: *Please comment on the statistical approach used by the EPA for developing the draft EEMs for broiler confinement houses and swine and dairy lagoons/basins. In addition please comment on the approach for developing draft EEMs for egg-layers, swine and dairy confinement houses.*

Section 7 of Broiler Report: DEVELOPMENT OF EEMS FOR GROW-OUT PERIODS

Current Approach

The Panel understands that EPA needs a method to routinely estimate air emissions on animal feeding operations.

The statistical models need to contribute to the goal of developing models to make accurate predictions on farms across the US.

The data used for the statistical approach cannot be assumed to represent other farms in the US and therefore the multiple regression models are wholly inadequate to routinely estimate emissions on farms outside the dataset.

Alternative Process-Based Model Structure

EPA should develop a process-based modeling approach to make predictions of air emissions on farms. Statistical methods should be used to fit parameters for models based on mechanisms of processes, and for evaluation of models.

The EPA should develop process-based models or other biologically driven models of different levels of complexity as needed. For example, a very simple model with only a few variables (e.g. number of animals, stage of growth, surface area, production rate) could be used to roughly estimate emissions on different farms. More complex models including additional variables (e.g. manure composition, feed composition, weather or climate parameters) could be used when more accurate estimates are desired.

The alternative structure will be simpler and more easily developed than the multiple regression approach.

Certain variables should have been considered and included in the parameters considered in the current modeling approach. All relevant variables were not used. More consideration to mass balance and process-based models is needed. Diets can have a large impact but are not included in the parameters considered in the current modeling approach. Table 7-2 parameters are apparently based on chemistry and knowledge of animal systems. Air flow, temperature, and time variables are related to chemistry. However, feed rate and composition, water management, and manure composition (moisture and N) also relate to the chemistry. These and other factors outside of the control of the EPA model builders should probably be collected in one place, and should be incorporated into the model. Season is not in the model. The data cover somewhat

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different time periods. It may however be difficult to include season in a simple manner. The California sites are sampled from Sept 2007-Oct 2009 while Kentucky sites were sampled from February 2006 to March 2007. There is, thus, some confounding between location and time of sampling (year of sampling). This may affect inference for seasonality. A relevant variable that should be included is the nitrogen inputs.

Although it may not be possible to include these variables in the model, the EPA should be aware that if these variables are important, then predictions from the EEM might be limited.

Some of the variables exhibit measurement error (number of birds and average bird weight are estimates). Consider accounting for the error because if it is not accounted for the relationship between the concentration and predictors is attenuated.

Existing data from other studies can also be used. For example, studies on physical or biological processes can be used to develop equations that can lead to predictions.

Models must capture control factors. Otherwise, it would not be possible to identify or reward use of control strategies. For example, if a producer changes the diet for his herd, it can decrease ammonia emissions. Measurements in manure, diet or even milk can capture the changes and model estimates of ammonia emissions can reflect the change.

Model Evaluation

Model-development efforts should be iterative with model evaluation. With each improvement or addition of complexity to a model, the model should be evaluated against it predecessor.

Models should be evaluated using techniques of sensitivity analysis, boundary value analysis, and accuracy (model prediction error).

Regression analysis of predicted vs. observed should be replaced with regression of residuals. R^2, slope and intercept should be replaced with model prediction error, mean bias, and slope bias.

The collected NAEMS data should be used for model evaluation of the process-based model. This data may also be used to improve parameter estimates of the process-based model.

Data Needs:

It would be useful to distinguish between comments about the appropriateness of the data and the appropriateness of the statistical methodology at this point.

 The data are questionable, as has already been noted by many. For starters, the two establishments (CA and KY) cannot be plausibly assume to represent the US broiler production. At some point, it will be important to randomly sample establishments from the population of broiler producers, hopefully using stratification by factors such as size of the operation, location, etc.

Statistical Modeling Approach

1. The panel recommends the EPA develop a modeling approach that is more consistent with the sampling design structure and data limitations. Model development needs to consider effects of location (site or farm), house within location, and flocks within house in model inference and prediction. Model uncertainty needs to recognize the limitations in using a small number of locations. The panel is concerned that any model developed from information on two sites is not applicable to all sites in the US.

2. The panel further recommends the EPA carefully consider revising the process for developing the statistical model, paying further attention to the mean and variance components of the model. In particular, the approach for evaluating random effects requires attention. The panel also expressed concern about using a polynomial model for estimating the relationship between animal mass and concentrations. It would also be helpful to decide what EPA has to predict in each time period. The appropriate statistical methodology may be quite different.

3. The panel recommends that residual analyses have more importance in the report and modeling process. It is preferable to plot residuals to look for oddities, lack of fit, serial correlation and lack of support for the probability model rather than histograms of the data. The mean and variance specifications should be assessed in an extensive analysis of residuals. The covariance structure, including the likely contemporaneous correlation among residuals for different houses at a single site, should also be assessed using the same residuals.

4) The panel recommends the EPA consider other approaches to the validation method used to evaluate model predictions. K-fold crossvalidation methods are preferable to simple data splitting.   Splitting of data based on factors related to study design (such as flock, house and location) should be considered as a way to evaluate model predictive ability.

General comments

1. The modeling approach suffers from largely ignoring the sampling/design structure of the data and implications. The model development process, with an overemphasis on p-values of predictors, would suggest that the primary goal might be inference rather than prediction.   The sampling design determines the ability to make statements about the collection of potential samples. In this design, there are locations (sites), houses within locations, and flocks within houses. These design factors are are not represented in the final models presented and the flocks factor is ignored in the modeling process. They are fundamental when it comes to making inferences about what factors and interactions are important as they affect the variance estimates and degrees of freedom for testing. While it would be useful to add factors associated with year and season, we suspect that the imbalance in the data will cause limitations when the model is applied to new sites. The importance of factors such as location have been reported in the literature (Ogink et al, 2008, Mosquera and Ognick, 2004)

Ogink, N.W.M.; Mosquera Losada, J.; Melse, R.W. (2008) Standardized testing procedures for assessing ammonia and odor emissions from animal housing systems in The Netherlands In:

Proceedings of the Mitigating Air Emissions from Animal Feeding Operations Conference, Des Moines, Iowa, USA, 19 - 21 May, 2005. - Des Moines : Mitigating Air Emissions from Animal Feeding Operations Conference, 2008-05-19/ 2008-05-21

Mosquera, J. and N.W.M. Ognik. 2004. Determination of the variation sources associated with ammonia emission measurements of animal housings. AgEngr 2004. Leuven, Belgium.

There is a fundamental problem with any attempt to extrapolate inferences or predictions to sites other than the three sites represented in the NAEMS dataset. The EPA attempts to resolve this problem of inadequate sample design by combining the information from separate sites into a single data set, hoping that a single model without site factors may be useful for predictions not only at these 3 sites but at other sites in other states. While it is helpful to combine the sites for assessing the value of the predictors in model building, inferences are likely limited to the locations and houses that are available. N=3 sites is an extremely small sample for developing models for use in other locations. An estimate of a variance component for random site effects, necessary for realistic uncertainty measures in predictions for other sites, would be highly unreliable with so few sites.

2. The process of developing the statistical model for predicting each pollutant should begin with finding appropriate specifications of:
- o   the mean, as a function of the predictor variables;
- o   the variance, as a function of the mean and/or the predictor variables.

These issues are addressed in the current draft report. However, the distributional form of the observations, identification of which is the first step in the process described in the Draft, is generally accepted as less important than the mean and variance specifications. The panel expressed concern about the both deterministic and stochastic components of the model. Specifically

- Nonlinear models: Polynomial regression, such as the use of cubic functions to represent nonlinear dependence in average mass of animals, can lead to poor predictions near the extremes of the experimental conditions, and to disastrous extrapolations only just beyond those extremes. The model results should indicate the values that might occur for maximum bird mass.   The restriction on the range of average mass should be reported if the cubic model is used. Plots of individual flocks suggest that different models might be appropriate for different flocks or that a random effect due to flock is needed. Some alternative strategies to polynomials for nonlinear relationships might be considered. For example, one could use low degree of freedom splines that are linear at the boundaries. If polynomials are to be used, the panel recommends use of orthogonal polynomials. With these one can arguably consider simpler final models by eliminating some interaction terms rather than keeping all three polynomial terms in any interaction considered.

  Some additional issues with EPA's regression modeling approach include:
  - o   The response variable is censored and this ought to be accounted for in the methodology.

- o Some of the predictors (e.g., number of birds in the house and average bird weight) are measured with error. If this error is not accounted for when fitting the model, then the relationship between the response and the predictors is attenuated.
- o There must be correlation across flocks housed in the same house and also across houses in the same establishment. Flocks need to be included as random effects in a model so that the "clustering effect" of house and establishment can be accounted for.
- o Even with these limited data, the variance component corresponding to house was highly significant (see Table 7-8). It is not clear to me why the EPA analysts declared it to be not significantly different from zero. When more houses are included in the sample, it will be very important to allow for house to house, flock to flock, and even establishment to establishment variability. It may not be there, but the judge is still out on this particular issue due to the scarcity of the data at this point.
- o The fact that the R^2 coefficients are so high is promising, but one should notice that this may well be due to the fact that a limited set of data are used to fit the model.
- o Residual plots should be presented.
- o There is clear lack of constant variance. As is common in data of this kind, the variance and the mean are correlated, so that, e.g., the variance in the response increases as the mean response also increases. A simple solution to this problem is to transform the response variable since transformation sometimes disentangles the mean and the variance. One possibility is to just use a square root of a log transformation (assuming that we report the zeros as censored).

- Correlation structure: It is not clear that the very high temporal correlation structure has been adequately modeled. Common time series tools (ACF and PACF) should be considered to assess the adequacy of the AR(1) model. The defense of the current model seems to be based entirely on the coverage of predictive intervals. While this is important, this does not guarantee a good model (overall coverage near 95% does not necessarily mean that coverage conditional on other factors is also 95%). The extremely high autocorrelation suggests that perhaps there are some other temporal trend features that could/should be identified.

- Random effects: The analysis approach must consider random effects for flocks. It is possible that other factors (such as buildup) may account for most of the flock effects, but it is still necessary to consider a flock random effect to account for what must be considered dependent observations (beyond the temporal dependence). Although house and location are also considered as potentially random, there are too few levels of the house and site factors to analyze them as random effects. They should be modeled and tested as fixed effects. We would hope that the house and site factors would act like additive blocking effects in addition to other predictors, but it could be necessary to consider interaction effects permitting other predictors to have different coefficients at different sites.

3. Crossvalidation is a useful tool for model selection and for evaluating predictive ability. Its value is constrained by the method for selecting the test set for model evaluation. By selecting a random sample of observations, as was done in this study, the results concerning predictive ability are limited. It is unlikely the method as applied in the EPA report will give a good measure of the predictive ability for a site in Florida, or another state or another location within Kentucky. It should however be possible to estimate prediction error for different flocks, for different houses and for different locations by running exercises using these factors to select holdout samples. The crossvalidation exercise could help identify the limitations to the model and to obtain a better estimate of the prediction error at new locations or new flocks. Even with the available data, crossvalidation may not inform about the reliability of predictions for sites in other states, or even other sites in Kentucky.

The exercise described in the Draft as "cross-validation" is not what most statisticians understand by that description. Five-fold cross-validation would involve a similar division of the data set into fifths, but each would be held out in turn, and predicted using a model fitted to the other four fifths. We suggest consideration of a leave-out-one-flock-at-a-time crossvalidation strategy. It would be helpful if EPA provided more information on the likelihood that observations from successive flocks might be nearly independent, and whether flock-to-flock variability vs. daily predictions is the fundamental variance component for inferences.

The study design involves location, houses within location and flocks within location. It is not likely that flocks are independent since all the flocks within a house are maintained under similar conditions. Conditions between houses are likely to be somewhat different so flocks from different houses should be less similar. Note that the greatest dependence is likely to be between measurements within a flock as the measurements are made over a short time period.

The exercise described in the Draft is also not a true validation, because the performance of candidate models in predicting the hold-out data was used in the model selection process. In a true validation, the test data would be held out of the entire model selection and estimation process. Model and analysis must incorporate the factors in the experimental design. That is, the "house", "site" and "flock" factors must be part of any analysis.

In fact, the panel thinks that an interesting exercise would be to build an EEM model on just one site (or perhaps the pair of sites in Kentucky) and examine how well the predictions apply to another site. This is severely restricting the amount of data available for modeling, but if predictions were good in this assessment it would lead to some hope that the model could actually be applied to other sites.

4. The panel recommends that residual analyses be part of the report. Histograms are used to indicate that the data are skewed; however, these plots are rather limited, as the authors point out. It is preferable to plot residuals in order to look for oddities, lack of fit, serial correlation and lack of normality. The mean and variance specifications should be assessed in an extensive analysis of residuals. Table 7-9 is definitely not a good way to assess mean-variance relationship as the constant range of NH3 values in the rows of the table constrain the SDs to be similar. The covariance structure, especially the likely contemporaneous correlation among residuals for different houses at a single site, should also be assessed using the same residuals.

In addition to normal QQplots and the overall plots of residual plots vs fitted value, we strongly suggest that residuals (and/or validation prediction errors) be broken down and examined according to spatial and temporal design factors. For example, boxplots of residuals should be made by site, house, flock, and season. We also suggest time series plots of observed and fitted (or predictions in the case of cross-validation) emissions separately for each of the five houses at the 3 sites.

5. The variable selection approach in the model building is likely suboptimal with respect to the goal of accurate prediction. We would recommend a modern text focusing on prediction, such as "The Elements of Statistical Learning" by Hastie, Tibshirani and Friedman. Because the primary aim is prediction there is no reason to base variable selection on backward elimination with a conservative p<.001 criterion.   The apparent significance of individual predictors is not a primary concern, especially in the context of (somewhat) correlated predictors. We don't know any justification for making decisions about inclusion of sets of interaction terms on the basis of a small change in R^2. While the final choice of model was not completely automatic according to the backward elimination algorithm, there seems no reason not to consider the results of an all subsets regression procedure rather than backward elimination (although this might only be possible without all the interaction effects) using a BIC criterion. Uncertainty in the "best" model could be assessed with cross-validation (see below).

Miscellaneous:

Page 7-29 Bottom of second paragraph - centering does not produce data where 50% are below zero and 50% above unless you are centering by the median.

Page 7-37 (2nd paragraph) Three sites, two in Kentucky and one in California, cannot be considered representative of all sites sites of interest in these and other states? Consider rewriting the sentence.

Figure legends could contain more information. For example, Table 7-16, mention this is standardized data.

The use of the regression of predicted versus observed is potentially difficult as one may obtain an R^2 of 1.0 when there is a biased model.

Check calculations of LL and BIC - these seem to be based on REML rather than ML

We don't believe that one should be trying to test the significance of the variance component for house when there the only replication of houses is the case of 2 houses in California, but we note that in Table 7.8 it appears that the variance component for house is significant (or this is a typo).

It might be useful to consider a method such as quantile regression for estimating the percentiles of the distribution rather than the average values. It would be helpful if EPA provided more information on the merits of such regression analysis for this project in contrast to the current notion of reporting uncertainly intervals on point predictions.

Despite the authors belief otherwise, we believe that there is evidencs of <u>lack of constant variance</u>. As is common in data of this kind, the variance and the mean are correlated, so that, e.g., the variance in the response increases as the mean response also increases. This is especially clear for some of the outcomes plotted in section 8. A simple solution to this problem is to <u>transform</u> the response variable since transformation sometimes disentangles the mean and the variance.

Table 7-3. Note that more than half of data is missing in fall, 79% missing in California.

Centering and scaling the predictor variables (usually termed "standardization") has no effect on collinearity, except between a predictor and the constant term. However, centering and scaling the predictor variables can improve numerical characteristics of the design matrix for computation. The Panel suggests that EPA consider an orthogonal polynomials approach, as noted above.

When a model estimated using "base" data is evaluated by comparing its predictions for "hold-out" data, the rmse (root mean squared prediction error) is the most important summary. The R^2 for the regression of the hold-out data on the predictions is less relevant as it involves a correction for any systematic bias due to a nonzero intercept and slope different from one; testing that the regression has a slope of 1 and an intercept of 0 gives some information about possible differences between base and hold-out data.

In Section 7.4.3: "a small p-value indicates that the estimated value of the parameter is not significantly different from zero " is presumably a typo as it is the opposite of the correct interpretation; a small p-value indicates that the estimated value of the parameter *is* significantly different from zero.

There is a lack of data/modeling of correlation between houses on a farm which is necessary in order to put confidence limits on a total farm emission estimate. Future data collection should include information on multiple houses. The report shows concern at the end of section 7.4 (p. 7-37) for making predictions at sites not included in the NAEMS. Unfortunately, if there are any significant differences between the sites available, whether in variance and auto-correlation parameters or other fixed effect parameters, any such predictions cannot be justified. It is a limitation of the study design that collected data on only 3 sites in 2 states. One cannot ignore heterogeneity across sites and rely on predictions assuming no heterogeneity, as suggested at the end of section 7.4.

Consider a joint test of significance of the slope and intercept in the model that compares predictions and actual values (p 7-42).

Finally, one additional comment that has to do with EPA having to produce a DAILY estimate and also an ANNUAL emission. For the annual estimate, the standard regression approach is fine. But for the daily estimate, if what EPA needs is a maximum (or something along those lines) then we need to be talking about working with QUANTILE REGRESSION, which directly predicts, for example, the 95th percentile of emission for the day, with its own standard error.

Charge Questions 5 and 6 Response

Charge Question 5*: Please comment on the EPA's approach for handling negative or zero emission measurements.*

Charge Question 6: *In the interest of maximizing the number of available data values for development of the draft H_2S EEMs for swine and dairy lagoons/basins, does SAB recommend any alternative approaches for handling negative and zero data other than the approach used by the agency.*

Summary: There are two types of negative values – raw concentration data and calculated concentration differences. Calculation of concentration differences (outlet minus inlet) can create negative emission rate estimates; negative concentrations may or may not lead to negative emission rate estimates. For both the raw concentration data and the calculated concentration differences, there was a diversity of Panel opinion on whether EPA should use negative and zero values in calculating EEMs. Panel members raised the following points without reaching agreement on whether to keep or discard zero or negative data:

Keep all zeros and all negative values.

- **Calculated data:** Zero and negative values should be included because:
    - If the calculated value is 0, it should be used. The Panel reached consensus agreement on use of these zero values.
    - Background values, used to create the calculated values (measured – background), were measured either intermittently (twice a day for gas), or continuously without correction for lag time in the barn (PM data). This could lead to a bias either up or down, potentially creating negative data values.
    - If an event occurred outside the barn (i.e., other barn cleanout, manure movement, etc.), or meteorological conditions created the exhaust air to come back into the barn, these events may create a spike or change in measured values that effect the calculated values.
    - If negative values are excluded due to calculated error, then there is a bias toward those values that were overestimated on the positive side (these values were not taken out of the data set). The average value should be zero. Standard deviation is half positive, half negative. The true estimated value would be closer if all estimated values were included.
    - Negative emissions also had high QA, and there is reason why they washed through.
    - If the calculated value is negative, the raw data can be consulted to discover if it is a calculated effect or other.
    - Relatively small number of data points were negative. Negative data does not appear regularly on a daily basis. Seem to be small offsets.

- o Generally can estimate uncertainty with those negative values.
- o If you build a model to make predictions, and the model excluded negative values, the model will be biased when predicting at low emission rates. Any bias in the model weakens the case for use of the end product.
- o There is already a lot of uncertainty in the measurements, which speaks to inclusion of negative values that qualify.
- o There is no statistical problem with inclusion of negative values into the model.
- o If negative rate was due to negative measured rates, go to one half of minimum detection limit (MDL), and include them.If we know the minimum detection level of the instrument that made the measurement, then any measurement below that detection limit is censored (something between 0 and the MDL) and should be treated as such in the analysis. This would include any value below the MDL, including negative values, zeros, etc.

- **Raw data.**
  - o If the raw data is 0 after instrument calibration adjustment, it should be used. The Panel reached consensus agreement on use of these zero values.
  - o If the instrument produces a negative concentration value that is due to a "below detection" or "minimum detection limit (MDL)" reading, but within instrument limits, the number should be used. Suggestions on the use of negative values from instrument:
    - Convert negative value, that is within the instrument error to 0 and use.
    - Use the negative value produced if it is within instrument error. Often times values fall below the standard curve as part of the variation of equipment, error, etc.
    - Use EPA procedure of using half of the MDL when observed value is below limit of detection.
    - Outliers should be treated per the QA/QC process first outside of this process, then assessed for negative and zero effects based on above criteria.
  - o If raw data is deemed negative after adjustment due to calibration, the value should be included in the data set. If not, there is a bias to those data that are positive due to the same process.

Use some zeros and negative values.

- Data should be qualified on an individual basis.

- Don't make blanket statement. Consider including negative values in some cases. Go element by element. There also may not be a situation/statement that applies for one compound under all circumstances (e.g., due to differences in background concentrations depending on location).
- Raw negative data should be qualified, and considered.

4/5/12 Preliminary Draft Comments for Deliberations of the SAB Animal Feeding Operations Emissions Panel Review of EPA's draft Emissions Estimating Methodologies for Broiler Operations and for Lagoons and Basins at Swine and Dairy Operations. Please Do not Cite or Quote. These comments are preliminary and do not represent SAB consensus comments nor EPA Policy.

Exclude zeros and negative values.

- If the measured concentration value is below lowest detection limit for the instrument *and* out of instrument error, limits, or uncertainty, then the value should be removed from data set. Qualify data individually.
- If there is instrument drift, ok to not include. Majority of negative values for H_2S EEMs for swine and dairy lagoons/basins were with instrument drift.
- Observed data should not be negative and *any* negative data is not good data and should be considered for elimination.
- If negative value is outlier, then OK to exclude.

Information needs:

- Consider whether raw, unqualified data should also be presented on EPA website.Need description of origin of zero and negative values. Add clear definitions in a table.

- Clarify why EPA checked negative measurements.

- Clarify whether all negative values for Lagoon Report were thrown out, or screened and selectively used.

- Clarify how EPA handled negative values for lagoon document. Discuss what drove negative values in this set of data. Drift?

- Prepare an outlier analysis. Get information on how outliers were handled, and provide a better description on what the negative is.

- Discuss whether all observations were treated in the same manner; if large results were received, were they subject to similar QA/QC.

- Regarding how negative results arise: Pure measurement error vs. anomalous events should be differentiated. It would be helpful if EPA provided more information on whether an event outside the barn was sufficient reason to invalidate a calculation.

- Report accuracy of ventilation rates, wind blown events, concentration data. Calculate uncertainty of these conditions.

Alternative approaches.

If model is not right shape, can do linear regressions. The magnitude of error is percentage error. If percent is true value, this is a multiplicative error. That error may be a small component of overall regression model. If small number of zeros, that is significant. If have negative value where error ends is different if negative error when hit zero.

There are general methods available to fit non linear models with negative values. There is no statistical problem with fitting such values, and No methodological reasons for excluding negative values. It may be important to fit negative values for these emissions. If truncate model at zero, you may be turning a linear into a non linear model.

Charge Question 7 Response

Charge Question 7: *Please comment on the approach EPA used to develop the draft broiler VOC EEM.*

The Panel identified significant limitations with the broiler VOC data, and concluded that the broiler VOC data do not support generating a broiler VOC EEM at this time. However, there are valuable components of the VOC data that should be used as appropriate. The methods used to collect the VOC data need to be more extensively documented.

EPA is required to provide an EEM for daily and annual VOC emissions; however, there is provision in the Consent Agreement that if the SAB decides that the available data are not adequate to support development of the EEM, the EPA can delay that development until adequate data are available.

The limitations of the broiler VOC data include:

- VOC data is difficult to gather, and data is not available to support a sound prediction of VOC emissions.
- Canisters were used to sample VOCs, and canisters only assess certain type of VOCs; would need to use other techniques to gather other VOCs that canisters cannot collect.
- Two separate instruments were used to collect VOC data, using two different methods, with two different levels of data completeness.

CA VOC Data:

- The procedure used to collect VOC data in California has not produced useful data for empirical model development and should not be used in the EEM.
  - Used THM analyzer; did not use FID. Tried to use a photobooster analyzer, but resulted in bad data.
  - Did not do measure total VOC.

KY VOC data:

Based on EPA's presentation on KY VOC data, that data appears generally valid and usable. Concerns include:

- KY VOC data is a very limited data set, and thus concerned about applying it across USA as representative of VOC emissions.
- Unknown recovery rate from the canister. In the lab, was not able to get all compounds out of electropolished canister onto sorbent tube.
- Seven quarters of sampling were conducted. At each sampling event, four samplers were sent to a facility, with two placed at outlets at each barn. Concern is inlet samples were not taken.

Valuable components of the VOC data that should be used as appropriate include.

- Speciation data coupled with reactivity information provides some general information on broiler emissions.

If VOC data are used to develop an EEM, the Panel needs more information on how VOCs were measured, particularly at the Kentucky site.

- Need more information on what drives VOC emissions, particularly at broiler facilities.
- Reactivity of the VOCs included in the measure of non methane hydrocarbons is important and should be available for use with any EEM that is developed and applied to agricultural operations.
- Some indication of the relative magnitude of the VOC emissions from broiler facilities to background levels and other sources would be helpful information.
- VOC speciation data are important and should be described further. The individual compounds found should be reported for both the Kentucky and California sites.

  o Identify what compounds were measured for both the Kentucky and California sites and which compounds might be extractable from GC/MS.
  o The most important compounds should be identified. For example, list the top twenty VOCs that should be collected, and describe why these are the top twenty.
  o Discuss QA/QC procedures that might assess speciation.
  o Show total and speciated VOC data.
  o Identify what fraction of the total was speciated in the results.
  o Compare data to other available AFO data, and indicate whether the VOC numbers are really significant.
  o Note whether there are reactive VOCs. Reactive VOCs provide less confidence in the overall data.
  o Identify what fraction of total was speciated in the results.

Summary Points on Sections 1, 2 and 10 of the Broiler Report

Section 1 of Broiler Report: INTRODUCTION

Section 2 of Broiler Report: OVERVIEW OF BROILER INDUSTRY

Section 10 of Broiler Report: REFERENCES

Section 1: INTRODUCTION

Reports are on a historical timeline; not until much later in the report that we discuss data collect, measurement technique problems. We should reflect this up front rather than in later parts of the study. Identify the limitations in the document

Review of **Consent Agreement process and history should be updated** to include description of what actually evolved that is some cases is different than the original intent (section 1.1).

Development of a Process-Based Model was the primary focus of NAS recommendations so this whole report should also focus on the 'processes' behind emission rate (ER). It was discovered during discussion of this draft report that development of the process-based model is a long term EPA goal. If a process-based model is not the current intent of EPA effort, **the development of statistically-based models as short-term tools should be explicitly stated early in the report**. Even so, the report's analysis would be strengthened by referral to the mechanistic processes behind the emission estimating methods employed. Primary mechanisms that lead to emissions of each regulated parameter should be described in relation to the surrogate statistical parameter for a better understanding of how the statistical model is valid. For example, bird number and mass is considered a surrogate for fresh manure production that impacts ammonia emission.

Minor note: The Air compliance Agreement had a record number of participants at 2600 yet this is a very small fraction of the one-half million AFOs in the country (section 1.0). EPA may want to build a case that although only 0.5% of AFOs chose to participate that they represent xx% (hopefully a large fraction) of total confinement animal production.

NAEMS **data collection expectations** need to be established in section 1.2. Some listed parameters are continuous and some periodic and this difference in data collection guidelines was noted in EPA presentation slides. This section would benefit from similar treatment to let readers know that some items are grab samples while others can be collected full time. For each animal species report, be sure that methodologies listed and described matches what was actually used! Our panel noted discrepancies in instrumentation type listed here and noted as deployed later in the report. Note when data were not collected or not provided for final analysis even if collected; or more simply, leave irrelevant data parameters out of the report. This long list leaves a first impression that all parameters were collected (which they were not) and collected with similar level of intensity (which they were not).

The accurate determination of ventilation rate (VR) is a very important aspect of the NAEMS data collection in order to achieve representative emission data. **The determination of accurate ventilation rate should be given more prominence in the report** with a concise description of how this was achieved (page 1.4). There was a lot of care and work involved in obtaining on-farm VR at each NAEMS site and this should be recognized. Also note throughout the report a correction for proper terminology: "static pressure *difference*" between inside and outside the building is the driving force for ventilation air movement and not simply "static pressure".

The broiler data were collected at an **extremely limited number of study sites**, even for the NAEMS. This should be acknowledged in the introduction. There were four broiler barns on three farms, which is half the number of study opportunities than any of the other species (barns/houses in NAEMS included 8 layers, 9 dairy and 11 swine). The study houses were felt to be representative of current industry practice but will shortly appear outdated as this industry is already adopting newer technology.

Table 1.1 needs attention so that 'rates' have a time unit and 'per animal' or 'per area' is needed in some other cases. There is a mix of American and Metric units that offers confusion.

There must be a quantification of emission uncertainty and/or variability. Emphasize that EEM currently being developed by EPA will offer a point value along with a confidence interval that represents the expected and naturally-occurring variation in emissions. This is an important aspect of the emission estimation and eventual reporting. The presentation of EEM as only one value for a given set of circumstances would be incorrect.

The range of conditions under which the NAEMS-based EEMs can be used needs to be explicitly stated. For example over what ambient temperature range during grow out or litter management period between flocks. There should be cautionary notes about using the EEM outside of the range studied.

Section 2: OVERVIEW OF BROILER INDUSTRY

Section 2.5 mentions that ER will be measured from both confinement houses and manure storages (but not land application). **There is no mention in this report about stockpiled litter storage emission measurements** (litter being the combination of bedding and manure). But the NAEMS did measure ER between flocks in houses empty of birds. Strengthen this section by noting that broiler houses are commonly managed as both bird production facilities and as dry manure storage if litter is not completely cleaned out between flocks. So the between-flock emission measurements of houses managed with de-caked built-up litter may suffice as manure-storage data. Here is a good place in the report to strengthen the **tie to the process-based model** development since litter, through microbial degradation and natural chemical interactions, is an emission source for all the parameters measured.

Throughout the report, **the emissions from populated houses during grow-out and empty houses during litter management needs to be presented separately** since the house is managed very differently during these two time periods. It is correct to segregate the differential in emissions observed from fully cleaned out houses versus de-caked built-up litter houses.

Ventilation system and control operation needs more clarification, particularly inlet description and function.

Section 10:   REFERENCES

Ogink, N.W.M.; Mosquera Losada, J.; Melse, R.W. (2008) Standardized testing procedures for assessing ammonia and odor emissions from animal housing systems in The Netherlands In: Proceedings of the Mitigating Air Emissions from Animal Feeding Operations Conference, Des Moines, Iowa, USA, 19 - 21 May, 2005. - Des Moines : Mitigating Air Emissions from Animal Feeding Operations Conference, 2008-05-19/ 2008-05-21

Mosquera, J. and N.W.M. Ognik. 2004. Determination of the variation sources associated with ammonia emission measurements of animal housings. AgEngr 2004. Leuven, Belgium.

Summary Points on Sections 3 and 4 of the Broiler Report

Section 3 of Broiler Report: NAEMS MONITORING SITES

Section 4 of Broiler Report: DATA AVAILABLE FOR EEM DEVELOPMENT

- Great lengths to describe parameters that are not used. If there wasn't enough data then consider providing this information upfront and then stop talking about the influence of those parameters
- Use this new found space to better describe procedures and build reader's confidence in the data
  - Really need to know how many samples were collected at each time
  - Fan calibration procedures and frequency
  - Missing details such as how the change in purge time for first 4 months of gas sampling in CA was dealt with
  - Figures are helpful, well organized. Integrate sampler info into the section. What analyzer, what TSP equipment, etc.
  - PM sampling schedule and disproportion of PM10, PM2.5 and TSP samples
  - Explain what data were not received and why
  - Explain the 75% completeness criteria – why that value? What did the 25% of data include – uniformity in what it represents?
  - Would benefit from being cleaned up and more careful about how the sites are described. Ie. Inlet systems are poorly described. Some discrepancies between section and later on
  - Ventilation rate should be more carefully described to illustrate the lengths taken to conduct the work (i.e. FANS system and repeated calibrations).
- A low frequency of negative values does not convey good maintenance; need to convey that QAPP was followed using some other means
- Are data representative of the industry and the literature?
  - Table 4-3 H2S data is highly suspect for CA1-B; this also needs to deal with the CA non-methane hydrocarbon. The footnote is incorrect. Either make another column with one state on one side and on other side, or improve the footnote.
  - PM2.5 emissions range for CA (table 5-11) is much higher than others and range does not match the same data presented in table 5-12
  - Growers will routinely record bird weight – not really the case
- Data received during call – disconcerting how many studies were completely disregarded. Those data should be able to be used to cross validate the developed EEMs. Tables should reflect what data would be applicable to validation
  - Consider use of more of the identified data – suggest additional criteria that might be considered or use these data as a performance evaluation of the EEM

- o Under what regimes would the EEMs, developed under limited number of houses give accurate results. So test the EEM against other data that address these different regimes.

Summary Points on Section 5 of the Broiler Report

Section 5 of Broiler Report: NAEMS DATA PREPARATION

- Section 5 raises more questions. It is not robust enough to address concerns on data quality. For example, section 5.1, calibration of the equipment is not clear and how the equipment malfunction and data outlier was dealt with?
- Two emission data acquisition programs were used, but lack of specific descriptions of the systems.
- Section 5.3. About data completeness, 75% completeness criteria is confusing. Table 5-2 shows less than 75% data completeness.
- Two sites comparison: they are different. Statistical analysis of the significant difference is needed.
- At Kentucky site, there is no reason for missing data.
- Why collection of the data at different time is not clear.
- Tables 5-11 ~ 5-14. Units need to be cleaned and consistent. Mass/bird/day is more appropriate than mass/day.
- Background data need to be included
- See separate discussion on zero and negative values.
- Table 5-13: California emission range is very high, and need to be checked.
- Table 5-10: break it into two tables: grow-out and clean-out.
- The objectives of the data collection need to be reviewed to guide data preparation. From a process analysis point of view, key tangible variables need to be included.
- In the Section 5.1: more data need to be included: such as mass balance data, hourly or daily average data?
- In section 5.2: Criteria for EPA selection and drop of the data need to be presented
- Need to analyze the two site conditions to see if they can cover the variation ranges of the U.S. broiler production. More analysis on the rational to have the two sites is needed than simply present the data.
- 75% data completeness criteria: sample size based on sub-data variation analysis is need to determine the criteria for data completeness for each of the specific air emission.
- Literature data need to be included for emission range analysis and possibly for the EEM validation.
- It is unclear whether it is preferred to report the Median or average here as a summary measure. If the measurements are skewed, then the average may not represent the middle of the data as well as the median will.

Summary Points on Section 6 of the Broiler Report

Section 6 of Broiler Report: MEASURED EMISSIONS FROM BROILER OPERATIONS

- Consider what other variables are needed; text suggests there are seasonal influences but season was not in the model.
- Negative values should be included in data presentation.
- Comparison is qualitative in nature – need to include the statistical comparisons, including outliers, range and variability
- Emission are expressed in g/d – express on a mass basis or unit area basis in order to normalize between sites so one can compare between sites
- Compare values with published data
- Use of cycle day rather than date or flock age – structure graph so that you have grow out and clean out sections
- The qualified data that is presented on EPA website should be better characterized and noted with clear columns.
- Instead of using ambient temperature, use house temperature.
- Need to present seasonal influences in data.

Summary Points on Section 9 of the Broiler Report, and Response to Charge Question 1

Section 9 of Broiler Report: DEVELOPMENT OF DECAKING AND FULL LITTER CLEAN-OUT PERIOD EEMS

Charge Question 1: *Please comment on the statistical approach used by EPA for developing the draft EEMs for broiler confinement houses…. In addition, please comment on using this approach for developing draft EEMs for egg-layers, swine and dairy confinement houses.*

The SAB supports EPA's use of emission factors to estimate emissions from decaking and full litter clean-out operations at broiler operations, but the SAB recommends that EPA express emission factors in more appropriate units than those proposed in the February 2012 draft methodology.

- EPA proposes to estimate emissions by using an emission factors in terms of "g pollutant/kg-bird-day" multiplied by a calculation of litter buildup. These emission factors increase with increasing numbers of flocks (days) on given litter. An "infinitely increasing" emission factor **does not** match available data in the literature.

- Other research has shown that the nitrogen content of litter reaches a balance after 3 to 5 flocks.

    o During the first four of 18 flocks, Coufal et al. (2006) reported little correlation between nitrogen volatilization and average temperature ($R^2 = 0.27$)

    o After 3-5 flocks, nitrogen volatilization is highly correlated to average temperature ($R^2 = 0.88$ in Coufal et al., 2006).

    o Experience shows that after 3-4 flocks, most of the litter material is effectively composted and has reached capacity to retain any more nitrogen per unit mass, thus the mechanism regulating ammonia emissions changes at this point, and the pool of available ammonia remains relatively consistent.

- **Therefore, a more appropriate method of estimating NH_3 emissions (for litter on which $\geq$3-4 flocks have been raised) would be in terms of "mass of pollutant per unit mass of litter removed"** (e.g. lb NH_3/ton litter removed). For litter on which < 3-4 flocks have been raised, an emission factor for ammonia in terms of "g pollutant/kg-bird-d" may be appropriate (per EPA's approach).

- To our knowledge, no similar information exists for constituents of interest to EPA aside from ammonia. However, it is expected that similar generation mechanisms would govern emissions of other gaseous constituents, so a similar emission factor units would

be appropriate. PM emissions would be expected to correlate with the mass of litter handled and litter age.

- EPA proposed emission factors calculated based on three different estimates of birds weight (i.e. cumulative weight, total shipped weight, or maximum weight). Litter production (for $\geq$ 3-4 flocks on litter) or total mass of birds raised on litter (for < 3-4 flocks) should be based on cumulative mass of birds raised on litter, as:

    1. This is the unit most pertinent to quantifying litter production,
    2. Bird inventory numbers are regularly collected by producers, and
    3. Bird mass is well modeled and can easily be predicted using growth curves.
    4. The market weight of birds is variable across the industry and is not fully represented in the data collected.

4/5/12 Preliminary Draft Comments for Deliberations of the SAB Animal Feeding Operations Emissions Panel Review of EPA's draft Emissions Estimating Methodologies for Broiler Operations and for Lagoons and Basins at Swine and Dairy Operations. Please Do not Cite or Quote. These comments are preliminary and do not represent SAB consensus comments nor EPA Policy.

Charge Question 1 Response and Comments on Section 3 of the Lagoon Report

Charge Question 1: *Please comment on the statistical approach used by the EPA for developing the draft EEMs for broiler confinement houses and swine and dairy lagoons/basins. In addition please comment on the approach for developing draft EEMs for egg-layers, swine and dairy confinement houses.*

Section 3 of Lagoon Report: DATA AVAILABLE FOR EEM DEVELOPMENT

Fold in comments of industry description: recommendations from NAS and wording and goals from NAEMS study.   Need to provide a thorough edit of industry descriptions.

3.2 negative values –define how test was done to show negative values did not compromise eem.

Table 3-1 identify what data not received and why (communication between EPA/SA/etc.) to clarify missing data.

Table 3.2 What specifically do animal numbers represent? (milking cows, versus milking and dry, with or without heifers); Facility type and lagoon/basin. What part of the manure is collected on the dairy side (just parlor, also housing?—is there a way to define collectable cow units?

Results from EEM generated in this study need to be put in the context of the data in table 3-3.

75% within an hour and 75% within a day rule for data completeness was too stringent for open source data. Need descriptive stats to show that use of other data degrade results. Potentially qualify size of gap to deal with potential bias yet allow additional data if less than 74%. Important to be sure gaps are not at the same time of day.

N loading must be considered in a regression analysis.

A description is needed as to why there is 30 minute timeframe.

Additional Data Needs

Broiler report:

1) Paul Sampson: Mean variance relationships are not in document, nor is a comparison of diagnostic variance vs. means. Were other assessments conducted other than just normality?

If Amy has saved results of her current fitted models, she should be able to generate some residual analyses without much effort. In the case of the Broiler report, in addition to normal QQplots and the overall plots of residual plots vs fitted value, we strongly suggest that residuals (and/or validation prediction errors) be broken down and examined according to spatial and temporal design factors. For example, boxplots of residuals should be made by site, house, flock, and season. We also suggest time series plots of observed and fitted (or predictions in the case of cross-validation) emissions separately for each of the five houses at the 3 sites.

It would be helpful to see ACFs and/or PACFs of model residuals, but this is a little more than just a plot of existing data. All of these might be just for NH3. My bullet points for the Lagoons report currently request similar things:

· Suggestion: Boxplots of emissions by the many farm level categorical factors, perhaps separately for different seasons or levels of other factors.

· Diagnostics: the usual residuals vs fitted values, QQ-plots to assess distributional form, etc., but also, break down residuals by farm (hence by animal). However, also generate, separately for each farm, time series of measured and fitted or predicted emissions according to the model.

Dr. Nail: She can give residual plots.

2) Rick Kohn: How much data was eliminated due to incompleteness?

Dr. Nail: She can get get back to panel on this.

3) Deanne Meyer: Is there a summary table on detection limits for analytical methods?

Larry Elmore: Yes, it's in QAPP. Will identify where.

4) Dave Allen: Measurements were made of cleaned-out litter; where was sample taken in this litter? If you are going to do a mass balance it would be good to know how long after the litter was removed from the house the sample was taken.

4/5/12 Preliminary Draft Comments for Deliberations of the SAB Animal Feeding Operations Emissions Panel Review of EPA's draft Emissions Estimating Methodologies for Broiler Operations and for Lagoons and Basins at Swine and Dairy Operations. Please Do not Cite or Quote. These comments are preliminary and do not represent SAB consensus comments nor EPA Policy.

Dr. Heber: Would need to check SOP for where and how floor and blowdown samples were taken.

5) Peter Bloomfield: Table 7-13 on page 7-43: please clarify what is being shown, and what is shown in table and what should occur when eliminating a variable.

Dr. Nail: She can provide clarification.

6) Eric Smith: Table 7-8 on page 7-36. Please clarify - that the second entry (sigma squared h) is actually sigma squared, otherwise there is significant variance component due to house.

Check to see it the -2LL and BIC are based on REML or ML methods. If model building is of interest, it is better to report ML calculations.

Is bird mass an estimated quantity, if so, how many birds were weighted to estimate the mass? Was the same approach used in both locations?

What version of SAS was used and which procedure?

7) Dave Allen: Panel should consider providing advice on how EPA could use more data than was used in the report. Panel could suggest criteria for looking at additional data and how to use it.   Any particular criteria to specify?

8) Brock Faulkner: It would be helpful to know why certain percentages of data were disqualified in the first place. With that information, could specify criteria.

Larry Elmore: NAEMS data used by EPA to generate EEMS is presented on EPA's website at: http://www.epa.gov/airquality/agmonitoring/data.html.   This data has already been QA/QC'd and includes qualifications, and followed QAPP per the consent agreement.

9) Dave Allen: Let's further consider whether raw, unqualified data should also be presented on EPA website.

10)   Viney Aneja: Why did EPA check negative measurements?

        April Leytem: Was any method applied to identify and eliminate outliers (both negative and positive)?

Robin Dunkins: Will check and get back on this.

11) Ronaldo Maghirang: For the broiler report, provide estimates of uncertainty for the emission rates. Include estimates of uncertainty for calculated emission rates from RPM and bLS methods.

Lagoon report:

12) Dave Allen: Were all negative values for Lagoon Report thrown out, or were they screened and selectively used? How did EPA handle negative values? For broilers saw why; what drove negative values in this set of data? Drift?

 Dr. Nail: Zero or negative values from this dataset had different reasons for omission than in the Broiler data set.

Robin Dunkins and Dr. Heber: Not sure; will get back on this. In some situations, concentrations are low.

13)   Deanne Meyer: EPA should provide information on how outliers were handled, and provide a better description on what the negative value is.

        April Leytem: This is more important for the lagoon data.

14) Deanne Meyer: Since EPA assumed that lagoon volume capacity for static assumed same volume, EPA should describe lagoon shape (e.g., typical sides; straight vs curved; sloping shape; range of design shapes, etc.). .

Danny Greene: Will provide information on slope of lagoons.

15) Ronaldo Maghirang: Did RPM measurements have calculated uncertainty values (e.g., 10%? 20%?)

Danny Greene: Will provide information on that.

16) Robert Hagevoort: Lagoon Report, Section 3:

a) Table 3-1, page 3-3. What does 'not received' data mean. If data exists, should be reviewed. Clarify caption D regarding nitrogen. Conduct a nitrogen mass balance on this data.

b) Table 3.2: H_2S for IN5 data: clarify why average emissions are zero, and max daily as 42.9.

c) Clarify how much manure is captured in lagoons. Did all manure end up in lagoons?

d) Clarify whether solids separation systems are in place. Settling ponds? Solids separation?

17) Deanne Meyer: Lagoon Report, Section 3:

a) Discuss cow excretion data, what % of structures contribute to the volatile concentrations, and % of residence time manure is on hard surface.

b) Need table of when lagoon data was collected on each facility.

18) April Leytem: Provide scientific basis for model selection (RPM vs bLS). Both models may work equally well. If there is more data available using the bLS model discuss why you chose to not use that data. There was one validation study done (Ro et al., 2011) that compared the RPM and bLS model and found that the RPM over-estimated the emissions by 30% and the bLS model under-estimated by 2%.

Table 4-1. For WA5A and WI5A it says that there were no valid emissions days for NH3 using the RPM model, but in the final project report submitted to Dr. Heber there were 12 valid days worth of data reported for WA5A and 22 days for WI5A, what happened to that data?

Both Reports:

19) Deanne Meyer: Additional information needed on the reports we've reviewed in order to better understand what we've seen:

·   Description (preferably in table format) of which data identified in SOP were not received and why. Were these not collected,, collected and not submitted; collected but not required therefore not submitted? [needed for both studies]

·   The lagoon report assumes a constant surface area. This needs explanation or verification. Surface area can vary tremendously in structures with slope and considerable depth. If surface area is used to determine EEM then which surface area is used? Certainly, the structure is not full 365 days a year.

·   More direct estimates of manure and manure nutrient excretion and moisture content of litter are needed for the broiler study.

·   More direct estimates of total solids and nutrient loading to lagoons/basins are needed for the lagoon study. Collectible cow units may be helpful.

20) Lingying Zhao: We need data on nutrient contents of animal manure, feed, and animal products. A mass-balance analysis can be conducted using these data to verify if the modeling results are correct in bulk part.

In addition, as we suggested, hourly average data is useful for modeling, not daily average.

Additional Requests for Data:

a) Brock Faulkner: Table 4-1 shows MANY more "valid test days" for bLS modeling than it does for the RPM method, but a statement on p. 5-6 contradicts this. What is the data availability for bLS and RPM data?

b) Wendy Powers-Shilling: Clarify if milk production data were collected. It was my understanding part way through the study that every day bulk tank milk (in lbs) and dairy milk cow numbers was collected and recorded at the dairy sites.

Brock Faulkner: Dr. Heber stated in 2010 that he had milk production data for the dairies that were studied, but this data is not included in the dataset. Was this data collected? Was this data submitted to EPA? If not, why? This is standard data collected by producers.

c) Viney Aneja:

1. Was background data collected, and how was it utilized for the development of EEMs.

2. In the development of emissions for ammonia and hydrogen sulfide from water holding structures (i.e. lagoons and basins) for swine and dairy using the RPM model (Section 4.2) daily emissions were provided to US EPA by the NAEMS researchers. Continuous concentration measurements and meteorology data set should be provided, and the emissions be computed on a smaller time resolution as opposed to daily emissions.

3. The data for partially enclosed i.e. naturally ventilated housing for both swine and dairy was not discussed. This is an important data need as ~50% of all swine housing in NC is naturally ventilated.

4. The total nitrogen and sulfur content data of the lagoon and basin needs to be provided, and both of these should be used as static variables to determine ammonia and H2S emissions.

d) Al Rotz:

There were a couple issues related to the VOC portion of the document that could be added to the additional data needs.

1.   Better documentation of the measurement procedures used for monitoring VOC emissions. This should include the deviation from the initial procedures planned and why the procedures were modified. This could include a brief discussion on the difficulty of accurately measuring VOCs, strengths and weaknesses of the procedures used and justification for not using the data for developing EEMs.

2.   Documentation of the VOC species emitted from the facilities. This includes both the broiler houses and the manure storages. Even though the data are not sufficient for EEM development, the data are useful. Data on the compounds making up the total VOC measurement is useful for future work.